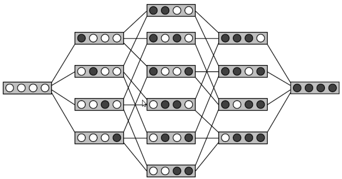
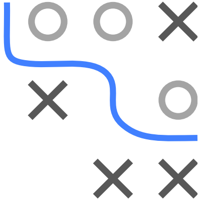
Supervised Learning

Wrapper methods

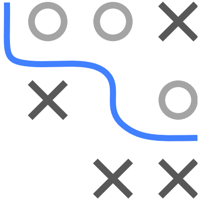




Learning goals

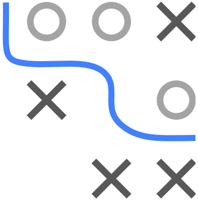
- Understand how wrapper methods work
- Understand how they could help in feature selection
- Know their advantages and disadvantages

INTRODUCTION



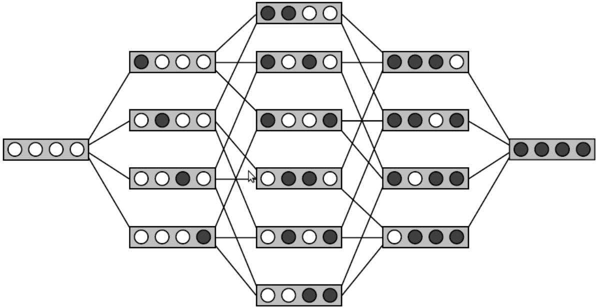
- Wrapper methods emerged from the idea that different sets of features can be optimal for different learners.
- Use the learner itself to assess the quality of the feature sets.
- Evaluation on a test set or resampling techniques are used.
- A wrapper is nothing else than a discrete search strategy for S, where the test error of a learner as a function of S is now the objective criterion.

INTRODUCTION



Wrappers have the following components:

- A set of starting values
- Operators to create new points out of the given ones
- A termination criterion

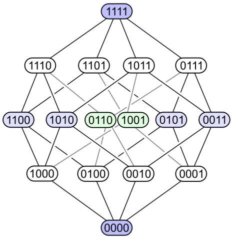


OBJECTIVE FUNCTION

Given p features, the **best-subset selection problem** is to find a subset $S \subseteq \{1, \dots p\}$ optimizing objective $\Psi : \Omega \to \mathbb{R}$:

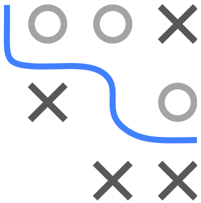
$$S^* \in \arg\min_{S \in \Omega} \{\Psi(S)\}$$

- Ω = search space of all feature subsets $S \subseteq \{1, \dots, p\}$. Usually we encode this by bit vectors, i.e., $\Omega = \{0, 1\}^p$ (1 = feat. selected)
- Objective Ψ can be different functions, e.g., AIC/BIC for LM or cross-validated performance of a learner.



Hasse diagram (source: Wikipedia)

HOW DIFFICULT IS BEST-SUBSET SELECTION?



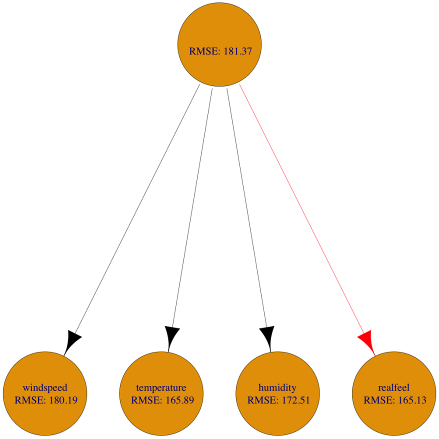
- Size of search space = 2^p, i.e., grows exponentially in p as it is the power set of $\{1, \ldots, p\}$.
- Finding best subset is discrete combinatorial optimization problem also known as L_0 regularization.
- It can be shown that this problem unfortunately can not be solved efficiently in general (NP hard; see, e.g., Natarajan, 1995)
- We can avoid having to search the entire space by employing efficient search strategies, moving through the search space in a smart way that finds performant feature subsets.

GREEDY FORWARD SEARCH

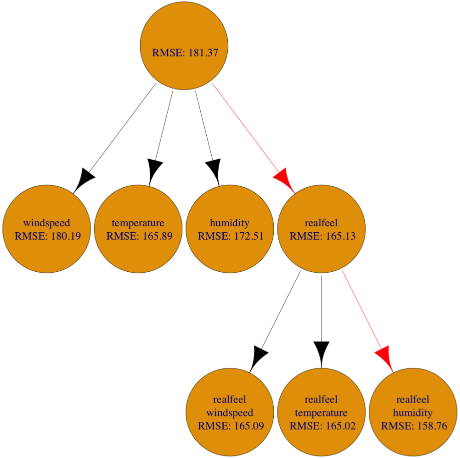
- Let $S \subset \{1, \ldots, p\}$, where $\{1, \ldots p\}$ is an index set of all features.
- Start with the empty feature set $S = \emptyset$.
- For a given set S, generate all $S_j = S \cup \{j\}$ with $j \notin S$.
- Evaluate the classifier on all S_j and use the best S_j.
- Iterate over this procedure.
- Terminate if:
  - the performance measure doesn't improve enough.
  - a maximum number of features is used.
  - a given performance value is reached.

GREEDY FORWARD SEARCH

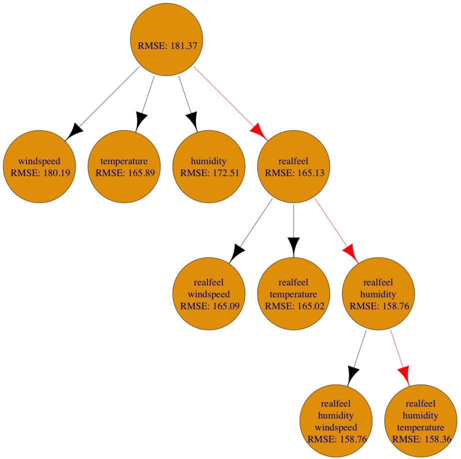
Example for greedy forward search on bike sharing data:



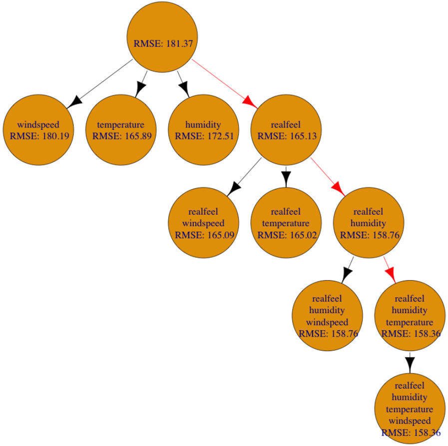
GREEDY FORWARD SEARCH



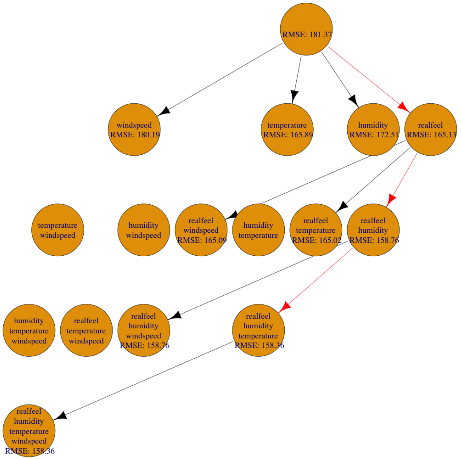
GREEDY FORWARD SEARCH



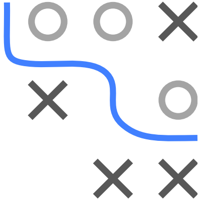
GREEDY FORWARD SEARCH



GREEDY FORWARD SEARCH

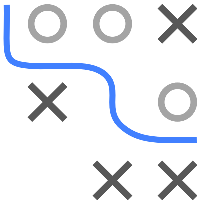


GREEDY BACKWARD SEARCH



- Start with the full index set of features $S = \{1, \ldots, p\}$.
- For a given set S generate all $S_j = S \setminus \{j\}$ with $j \in S$.
- Evaluate the classifier on all S_j and use the best S_j.
- Iterate over this procedure.
- Terminate if:
  - the performance drops drastically, or
  - a given performance value is undershot.

EXTENSIONS



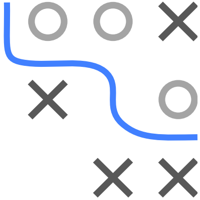
- Eliminate or add several features at once to increase speed.
- Allow alternating forward and backward search.
- Randomly create candidate feature sets in each iteration.
- Continue search based on the set of features where an improvement is present.
- Use improvements of earlier iterations.

EXTENSIONS

Algorithm A simple 1+1 genetic algorithm

Start with a random set of features S (bit vector b).
repeat
    Flip a couple of bits in b with probability p.
    Generate set S' and bit vector b'.
    Measure the classifier's performance on S'.
    If S' performs better than S, update $S \leftarrow S'$, otherwise $S \leftarrow S$.
until One of the following conditions is met:

- A given performance value is reached.
- Budget is exhausted.



WRAPPERS

Advantages:

- Can be combined with every learner.
- Can be combined with every performance measure.
- Optimizes the desired criterion directly.

Disadvantages:

- Evaluating the target function is expensive.
- Does not scale well if number of features becomes large.
- Does not use much structure or available information from our model.